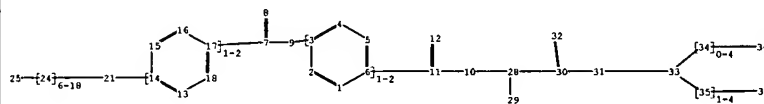
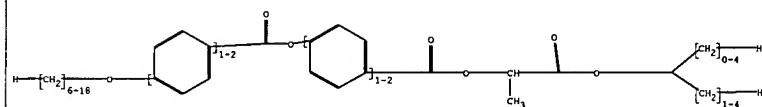


# WEST Search History

DATE: Wednesday, April 13, 2005

<b>Hide?</b>	<b>Set Name</b>	<b>Query</b>	<b>Hit Count</b>
		<i>DB=USPT,EPAB,JPAB,DWPI,TDBD; PLUR=NO; OP=ADJ</i>	
<input type="checkbox"/>	L5	L4 and l3	70
<input type="checkbox"/>	L4	@pd>20030101	3891712
<input type="checkbox"/>	L3	252/299.64	564
<input type="checkbox"/>	L2	liquid crystal\$ with swallow\$	36
<input type="checkbox"/>	L1	6740256 or 6245256	6

END OF SEARCH HISTORY



chain nodes :

7 8 9 10 11 12 21 24 25 28 29 30 31 32 33 34 35 36 37

ring nodes :

1 2 3 4 5 6 13 14 15 16 17 18

chain bonds :

3-9 6-11 7-9 7-8 7-17 10-11 10-28 11-12 14-21 21-24, 24-25 28-29  
28-30 30-31 30-32 31-33 33-35 33-34 34-36 35-37

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

3-9 7-9 7-8 10-11 10-28 11-12 14-21 30-31 30-32 31-33

exact bonds :

6-11 7-17 21-24 24-25 28-29 28-30 33-35 33-34 34-36 35-37

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom  
18:Atom 21:CLASS 24:CLASS 25:CLASS 28:CLASS 29:CLASS 30:CLASS  
31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS

RN 121169-71-9 REGISTRY  
 ED Entered STN: 16 Jun 1989  
 CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-(octyloxy)-, 4-[(2-butoxy-1-methyl-2-oxoethoxy)carbonyl]phenyl ester, (R)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1BC1ECPOPB  
 FS STEREOSEARCH  
 MF C35 H42 O7  
 SR CA

LC STN Files: CA, CAPLUS

DT.CA Caplus document type: Journal; Patent

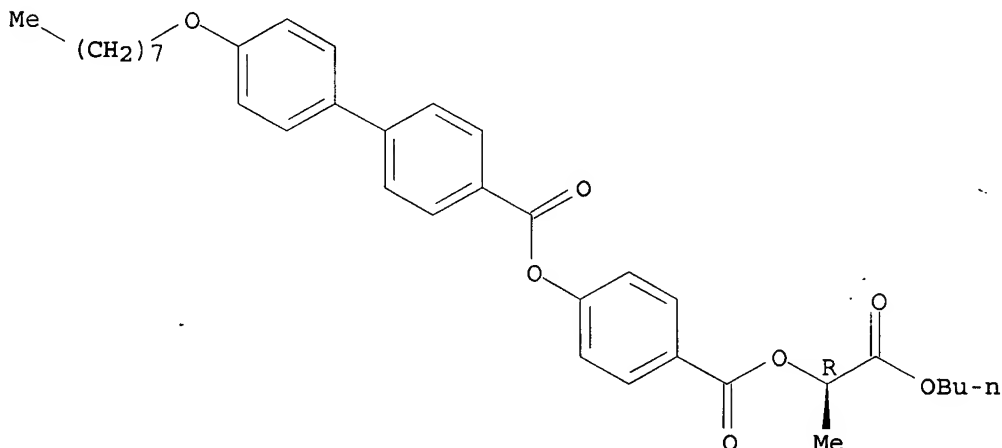
RL.P Roles from patents: PREP (Preparation); PRP (Properties)

RL.NP Roles from non-patents: PRP (Properties); USES (Uses)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
=====	=====	=====	=====	=====	=====
C6	C6	6	C6	46.150.18	3

Absolute stereochemistry.



*g* = 3  
=

Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1000000.0	pH 1	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 4	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 7	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 8	(1) ACD
Bioconc. Factor (BCF)	1000000.0	pH 10	(1) ACD
Boiling Point (BP)	695.0+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVP)	101.80+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	286.1+/-56.8 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	20		(1) ACD
H acceptors (HAC)	7		(1) ACD
H donors (HD)	0		(1) ACD

Koc (KOC)	10000000.0	pH 1	(1) ACD
Koc (KOC)	10000000.0	pH 4	(1) ACD
Koc (KOC)	10000000.0	pH 7	(1) ACD
Koc (KOC)	10000000.0	pH 8	(1) ACD
Koc (KOC)	10000000.0	pH 10	(1) ACD
logD (LOGD)	11.04	pH 1	(1) ACD
logD (LOGD)	11.04	pH 4	(1) ACD
logD (LOGD)	11.04	pH 7	(1) ACD
logD (LOGD)	11.04	pH 8	(1) ACD
logD (LOGD)	11.04	pH 10	(1) ACD
logP (LOGP)	11.042+/-0.481		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	574.70		(1) ACD
Vapor Pressure (VP)	3.64E-19 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software  
Solaris V4.76 ((C) 1994-2005 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

AN 122:240975 CA  
 TI Novel properties of conducting polymer-liquid crystal system and their doping effect  
 AU Kobayashi, K.; Yin, X. H.; Ozaki, M.; Kawai, T.; Yoshino, K.  
 CS Fac. Eng., Osaka Univ., Osaka, 565, Japan  
 SO Synthetic Metals (1995), 69(1-3), 597-8  
 CODEN: SYMEDZ; ISSN: 0379-6779  
 PB Elsevier  
 DT Journal  
 LA English  
 CC 36-5 (Physical Properties of Synthetic High Polymers)  
 Section cross-reference(s): 75, 76  
 AB Conducting polymer/liquid crystal systems of poly(3-dodecylthiophene) and poly(9,9-dialkylfluorene)s were prepared by casting from CHCl<sub>3</sub> solns. The ferroelec. liquid crystals used were (R)-4'-(1-butoxycarbonyl-1-ethoxy)phenyl-4-(4-octyloxyphenyl)benzoate (1BC1EPOB) and (R)-4'-(1-methoxycarbonyl-1-ethoxy)phenyl-4-(4-dodecyloxyphenyl)benzoate (1MC1EPDDPB). The structure of the system is strongly dependent on the concentration of liquid crystal and the mol. structures of the conducting polymer and the liquid crystal. Elec. properties such as dielec. response and optical properties are strongly dependent on the concentration of liquid crystal and correlated with the structure of the system. The conducting polymer/liquid crystal film did not degrade after repeated electrochem. doping and undoping cycles. A drastic change in absorptance [electrochromic effect] was observed upon doping, which is linked to insulator-metal transition of the polymer at high concentration of liquid crystal.  
 ST polyalkylthiophene butoxycarbonylethoxyphenyl dielec const;  
 electrochromism polydodecylthiophene octyloxyphenylbenzoate system;  
 conducting polymer liq crystal spectroelectrochemistry  
 IT Electric conductors, polymeric  
 Liquid crystals  
 (electrochromism and dielec. constant of conducting polymer/ferroelec.

liquid crystal systems)  
IT 86-73-7D, Fluorene, alkyl derivs., polymers 104934-53-4,  
Poly(3-dodecylthiophene) 121169-71-9 121169-72-0,  
(R)-4'-(1-Methoxycarbonyl-1-ethoxy)phenyl-4-(4-dodecyloxyphenyl)benzoate  
RL: PRP (Properties)  
(electrochromism and dielec. constant of conducting polymer/ferroelec.  
liquid crystal systems)

#### REFERENCE 2

AN 113:88106 CA  
TI Ferroelectric liquid crystals with large spontaneous polarization and high  
speed display devices  
AU Yoshino, K.; Taniguchi, H.; Ozaki, M.  
CS Fac. Eng., Osaka Univ., Osaka, Japan  
SO Ferroelectrics (1989), 91, 267-76  
CODEN: FEROA8; ISSN: 0015-0193  
DT Journal  
LA English  
CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other  
Reprographic Processes)  
Section cross-reference(s): 75  
AB Ferroelec. liquid crystals with a large, spontaneous polarization,  $>10^{-7}$   
C/cm<sup>2</sup>, were prepared by taking the following design factors into  
consideration: (a) separation between the chiral C and the dipole moment, (b)  
bulk of mol. group bonded to the chiral C, (c) introduction of large bond  
moments, (d) orientation of many bond moments around chiral the C, (e)  
dipole moment between the core and chiral C, (f) the dipole moment at the  
core, and (g) the effect of H bonds. Anomalous dielec. behavior in these  
new ferroelec. liquid crystals and high speed response times of < several  
tens of  $\mu$ s in electrooptic cells are discussed.  
ST ferroelec liq crystal display device  
IT Molecular structure-property relationship  
(electrooptic properties and spontaneous polarization, of ferroelec.  
liquid crystals)  
IT Optical imaging devices  
(electro-, liquid-crystal, ferroelec., with large spontaneous  
polarization)  
IT Liquid crystals  
(ferroelec., with large spontaneous polarization, effect of mol.  
structure on)  
IT Ferroelectric substances  
(liquid-crystal, of liquid crystals, effect of mol. structure on)  
IT 114880-36-3, 3EC2PCPOPB 115009-14-8, 1MC1ECPOPB 115021-88-0, 3B2PCPOPB  
121169-54-8, 2MC1PCPOPB 121169-71-9, 1BC1ECPOPB 122222-26-8,  
1MC1ECHOPOPB  
RL: USES (Uses)  
(ferroelec. properties and characteristics of electrooptic devices  
containing, spontaneous polarization and mol. structure in)

#### REFERENCE 3

AN 111:31748 CA  
TI Optically active benzene or biphenyl derivative liquid crystals  
IN Yoshino, Katsumi; Kitatsume, Tomoya; Sato, Kazuo; Yamazaki, Noritsugu;  
Taniguchi, Hiroki; Sagawa, Masahiro; Yaso, Isato  
PA Daicel Chemical Industries, Ltd., Japan  
SO Jpn. Kokai Tokkyo Koho, 27 pp.  
CODEN: JKXXAF  
DT Patent  
LA Japanese  
IC ICM C07C043-205  
ICS C07C043-225; C07C069-708; C07C069-734; C07C069-76; C07C069-82;  
C07C069-90; C07C069-92; C07C069-94; G02F001-137

ICA C09K019-08; C09K019-12; C09K019-20; C09K019-54

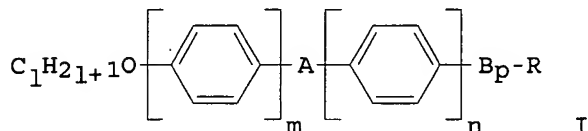
CC 75-11 (Crystallography and Liquid Crystals)

Section cross-reference(s): 25, 74

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 63307837	A2	19881215	JP 1987-190930	19870730
	JP 2562606	B2	19961211		
PRAI	JP 1986-209657		19860908		
	JP 1987-4090		19870113		
	JP 1987-7931		19870116		

GI



AB The title compds. I ( $l = 1-15$ ;  $m = 1, 2$ ;  $n = 0-2$ ;  $p = 0, 1$ ;  $A = \text{CO}_2, \text{OCO}, \text{CH}_2\text{O}, \text{OCH}_2$ ;  $B = \text{CO}_2, \text{O}$ ; when  $n = 0$ ,  $p = 0$  and  $A = \text{CO}_2$ ;  $R =$  optically active substituted alkyl) are prepared as ferroelec. liquid crystals. Treatment of 4-(PhCH<sub>2</sub>O)C<sub>6</sub>H<sub>4</sub>COCl with Me (S)-lactate in pyridine gave (S)-(+)-4-(PhCH<sub>2</sub>O)C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>CH(CO<sub>2</sub>Me)Me, which in EtOH was hydrogenated in the presence of Pd/C to afford (S)-(+)-4-HOC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>CH(CO<sub>2</sub>Me)Me. The latter was stirred with 4-Me(CH<sub>2</sub>)<sub>9</sub>C<sub>6</sub>H<sub>4</sub>COCl in pyridine to give (S)-(+)-I [ $l = 10$ ;  $m = 1$ ;  $A = \text{CO}_2$ ;  $n = 1$ ; BpR = CO<sub>2</sub>CH(CO<sub>2</sub>Me)Me], which showed a smectic A-to-isotropic transition at 45°.

ST liq crystal benzene biphenyl deriv

IT Liquid crystals  
(optically active benzene and biphenyl derivs.)

IT Optical imaging devices  
(electro-, liquid-crystal, compns. containing optically active benzene or biphenyl derivs. for)

IT 18520-63-3 121170-52-3

RL: PROC (Process)

